# Robust Summaries and Dossier for CAS No. 23500-79-0

| | | |
|---|---|---|
| **Existing Chemical** | : | ID: 23500-79-0 |
| **CAS No.** | : | 23500-79-0 |
| **Product name** | : | A-1846 |
| **EINECS Name** | : | 6-tert-butyl-3-(chloromethyl-2,4-xylenol |
| **Molecular Formula** | : | C13H19ClO |

**Producer related part**

| | | |
|---|---|---|
| **Company** | : | Cytec Industries Inc. |
| **Creation date** | : | 06.05.2003 |

**Substance related part**

| | | |
|---|---|---|
| **Company** | : | Cytec Industries Inc. |
| **Creation date** | : | 06.05.2003 |
| **Status** | : | |
| **Memo** | : | |
| **Printing date** | : | 29.05.2003 |
| **Revision date** | : | 06.05.2003 |
| **Date of last update** | : | 29.05.2003 |
| **Number of pages** | : | 27 |
| **Chapter (profile)** | : | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile)** | : | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile)** | : | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

### 1.0.1 APPLICANT AND COMPANY INFORMATION

### 1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

### 1.0.3 IDENTITY OF RECIPIENTS

### 1.0.4 DETAILS ON CATEGORY/TEMPLATE

### 1.1.0 SUBSTANCE IDENTIFICATION

### 1.1.1 GENERAL SUBSTANCE INFORMATION

### 1.1.2 SPECTRA

### 1.2 SYNONYMS AND TRADENAMES

**2,4-dimethyl-3-(chloromethyl)-6-tert-butylphenol**

**3-(chloromethyl)-6-(1,1-dimethylethyl)-2,4-dimethylphenol**

**4-tert-butyl-3-hydroxy-2,6-dimethylbenzyl chloride**

**6-tert-butyl-2,4-dimethyl-3-chloromethyl phenol**

**6-tert-butyl-3-chloromethyl-2,4-dimethylphenol**

**phenol, 3-(chloromethyl)-6-(1,1-dimethylethyl)-2,4-dimethyl-**

**phenol, 6-tert-butyl-3-chloromethyl-2,4-xylenol**

### 1.3 IMPURITIES

### 1.4 ADDITIVES

### 1.5 TOTAL QUANTITY

### 1.6.1 LABELLING

### 1.6.2 CLASSIFICATION

### 1.6.3 PACKAGING

### 1.7 USE PATTERN

**Type of use** : industrial
**Category** : Chemical industry: used in synthesis

**Reliability** : (1) valid without restriction
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### 1.7.1 DETAILED USE PATTERN

### 1.7.2 METHODS OF MANUFACTURE

### 1.8 REGULATORY MEASURES

### 1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

### 1.8.2 ACCEPTABLE RESIDUES LEVELS

### 1.8.3 WATER POLLUTION

### 1.8.4 MAJOR ACCIDENT HAZARDS

### 1.8.5 AIR POLLUTION

### 1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

### 1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

### 1.9.2 COMPONENTS

## 1.10 SOURCE OF EXPOSURE

## 1.11 ADDITIONAL REMARKS

## 1.12 LAST LITERATURE SEARCH

## 1.13 REVIEWS

### 2.1 MELTING POINT

| | | |
|---|---|---|
| **Value** | : | = 45 °C |
| **Sublimation** | : | |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | The melting point of 45 degrees C is for the pure crystallized substance. The product is usually isolated with 11-13% methyl isobutyl ketone (CAS No. 108-10-1) added to store and handle the product in liquid form (Cytec Industries, Inc. material safety data sheet dated 10/30/00 for A-1846). |
| **Reliability** | : | (2) valid with restrictions<br>Methodology was not documented. |
| **Flag** | : | Critical study for SIDS endpoint |

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| | | |
|---|---|---|
| **Value** | : | = -32 °C |
| **Sublimation** | : | |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | other TS |
| **Test substance** | : | The material is the commercially stored form containing 11-13% methyl isobutyl ketone solvent. |
| **Reliability** | : | (2) valid with restrictions<br>Experimental details were not provided. |

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### 2.2 BOILING POINT

| | | |
|---|---|---|
| **Value** | : | ca. 320 °C at 1013 hPa |
| **Decomposition** | : | |
| **Method** | : | other |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | EPIWIN Mpbpwin (v1.40) was used to estimate boiling point by the adapted Stein and Brown Method. Inputs to the model were CAS No. 23500-79-0 and the measured melting point (45 degrees C). |
| **Reliability** | : | (2) valid with restrictions<br>Data were obtained by modeling. |
| **Flag** | : | Critical study for SIDS endpoint |

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| | | |
|---|---|---|
| **Value** | : | = 156 °C at |
| **Decomposition** | : | |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | other TS |
| **Test substance** | : | The material is the commercially stored form containing 11-13% methyl isobutyl ketone solvent. |

**Reliability** : (2) valid with restrictions
Experimental details were not provided.
22.05.2003 (3)

### 2.3 DENSITY

**Type** : relative density
**Value** : ca. 1.044 g/cm³ at 20 °C
**Method** : other
**Year** :
**GLP** : no
**Test substance** : other TS

**Test substance** : The material is the commercially stored form containing 11-13% methyl isobutyl ketone solvent.
**Reliability** : (2) valid with restrictions
Experimental details were not provided.
11.05.2003 (3)

### 2.3.1 GRANULOMETRY

### 2.4 VAPOUR PRESSURE

**Value** : ca. .00018 hPa at 25 °C
**Decomposition** :
**Method** : other (calculated)
**Year** : 2003
**GLP** : no
**Test substance** : as prescribed by 1.1 - 1.4

**Remark** : EPIWIN Mpbpwin (v1.40) was used to estimate the vapor pressure by the Modified Grain Method. Inputs to the model are CAS No. 23500-79-0 and the measured melting point (45 degrees C).
**Reliability** : (2) valid with restrictions
Data were obtained by modeling.
11.05.2003 (10)

**Value** : ca. 12 hPa at 20 °C
**Decomposition** :
**Method** : other (measured)
**Year** :
**GLP** : no
**Test substance** : other TS

**Remark** : The vapor pressure conforms to that of the solvent.
**Test substance** : The substance is in liquid form, diluted by 11-13% methyl isobutyl ketone solvent.
**Reliability** : (2) valid with restrictions
Experimental details were not provided.
14.05.2003 (3)

### 2.5 PARTITION COEFFICIENT

| | | |
|---|---|---|
| **Partition coefficient** | : | octanol-water |
| **Log pow** | : | = 5.32 at 20 °C |
| **pH value** | : | |
| **Method** | : | other (calculated) |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | EPIWIN Kowwin (v1.66) was used to estimate the log Kow (Pow). Inputs to the model are CAS No. 23500-79-0 and the measured melting point (45 degrees C). |
| **Reliability** | : | (2) valid with restrictions<br>Data were obtained by modeling. |
| **Flag** | : | Critical study for SIDS endpoint |

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| | | |
|---|---|---|
| **Partition coefficient** | : | octanol-water |
| **Log pow** | : | = 3.9 at °C |
| **pH value** | : | |
| **Method** | : | other (measured) |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | other TS |
| **Test substance** | : | The material is the commercially stored form containing 11-13% methyl isobutyl ketone solvent. |
| **Reliability** | : | (2) valid with restrictions<br>Experimental details were not provided. |

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### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

| | | |
|---|---|---|
| **Solubility in** | : | Water |
| **Value** | : | = 10.19 mg/l at 25 °C |
| **pH value** | : | |
| **concentration** | : | at °C |
| **Temperature effects** | : | |
| **Examine different pol.** | : | |
| **pKa** | : | at 25 °C |
| **Description** | : | slightly soluble (0.1-100 mg/L) |
| **Stable** | : | yes |
| **Deg. product** | : | |
| **Method** | : | other |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | EPIWIN Wskow (v1.40) was used to estimate the water solubility. Inputs to the model are CAS No. 23500-79-0 and the measured melting point (45 degrees C). |
| **Reliability** | : | (2) valid with restrictions<br>Data were obtained by modeling. |

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| | | |
|---|---|---|
| **Solubility in** | : | Organic Solvents |
| **Value** | : | at °C |
| **pH value** | : | |
| **concentration** | : | at °C |
| **Temperature effects** | : | |
| **Examine different pol.** | : | |

| | | |
|---|---|---|
| **pKa** | : | at 25 °C |
| **Description** | : | of very high solubility |
| **Stable** | : | yes |
| **Deg. product** | : | |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | The pure crystalline substance can be liquified and dissolved into one liquid phase by adding 11-13% by weight methyl isobutyl ketone. |
| **Reliability** | : | (2) valid with restrictions<br>Experimental details were not provided. |

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| | | |
|---|---|---|
| **Solubility in** | : | Water |
| **Value** | : | = 500 mg/l at 25 °C |
| **pH value** | : | |
| **concentration** | : | at °C |
| **Temperature effects** | : | |
| **Examine different pol.** | : | |
| **pKa** | : | |
| **Description** | : | |
| **Stable** | : | |
| **Deg. product** | : | |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | other TS |
| **Test substance** | : | The material is the commercially stored form containing 11-13% methyl isobutyl ketone solvent. |
| **Reliability** | : | (2) valid with restrictions<br>Experimental details were not provided. |

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## 2.6.2 SURFACE TENSION

## 2.7 FLASH POINT

## 2.8 AUTO FLAMMABILITY

## 2.9 FLAMMABILITY

## 2.10 EXPLOSIVE PROPERTIES

## 2.11 OXIDIZING PROPERTIES

## 2.12 DISSOCIATION CONSTANT

### 2.13 VISCOSITY

### 2.14 ADDITIONAL REMARKS

### 3.1.1 PHOTODEGRADATION

| | | |
|---|---|---|
| **Type** | : | air |
| **Light source** | : | Sun light |
| **Light spectrum** | : | nm |
| **Relative intensity** | : | based on intensity of sunlight |
| **INDIRECT PHOTOLYSIS** | | |
| **Sensitizer** | : | OH |
| **Conc. of sensitizer** | : | |
| **Rate constant** | : | = .0000000000143539 $cm^3$/(molecule*sec) |
| **Degradation** | : | = 50 % after 8.9 hour(s) |
| **Deg. product** | : | |
| **Method** | : | other (calculated) |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | EPIWIN Aop Program (v1.90) was used to calculate the hydroxyl radical rate constant and half life. A CAS No. of 23500-79-0 was inputted. |
| **Reliability** | : | (2) valid with restrictions |
| **Flag** | : | Critical study for SIDS endpoint |

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### 3.1.2 STABILITY IN WATER

| | | |
|---|---|---|
| **Type** | : | abiotic |
| **t1/2 pH4** | : | at °C |
| **t1/2 pH7** | : | at °C |
| **t1/2 pH9** | : | at °C |
| **Remark** | : | EPIWIN Hydrowin(v1.67) cannot estimate a rate constant for molecules other than esters, carbamates, epoxides, halomethanes and specific alkyl halides. |

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### 3.1.3 STABILITY IN SOIL

### 3.2.1 MONITORING DATA

### 3.2.2 FIELD STUDIES

### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

| | | |
|---|---|---|
| **Type** | : | fugacity model level III |
| **Media** | : | |
| **Air** | : | .0002 % (Fugacity Model Level I) |
| **Water** | : | 11.6 % (Fugacity Model Level I) |
| **Soil** | : | % (Fugacity Model Level I) |
| **Biota** | : | 40.8 % (Fugacity Model Level II/III) |
| **Soil** | : | 47.6 % (Fugacity Model Level II/III) |
| **Method** | : | other |

| | | |
|---|---|---|
| **Year** | : | 2003 |
| **Remark** | : | Inputs into the EPIWIN Program were a measured melting point of 45 degrees C , a CAS No. of 23500-79-0, and an emission rate to air of 0 kg/hr. |
| **Result** | : | Half-lives in various media based on EPIWIN Biowin and EPIWIN aop are air = 17.88 hours, water = 1440 hours, soil =1440 hours, and sediment = 5760 hours. Biowin ultimate is estimated to be months. The EPIWIN Pckoc Program (v1.66) estimates the soil/sediment partition constant to be 1.705 E+4. EPIWIN Henry (v3.10) was used to calculate a Henry's Law Constant of 6.85 E-7 atm-m3/mole at 25 degrees C. |
| **Reliability** | : | (2) valid with restrictions<br>Data were obtained by modeling. |
| **Flag** | : | Critical study for SIDS endpoint |

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### 3.3.2 DISTRIBUTION

### 3.4 MODE OF DEGRADATION IN ACTUAL USE

### 3.5 BIODEGRADATION

| | | |
|---|---|---|
| **Type** | : | aerobic |
| **Inoculum** | : | |
| **Deg. product** | : | |
| **Method** | : | other |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | EPIWIN Biowin (v4.00) was used to predict biodegradability. A CAS No. of 23500-79-0 was inputted into the model. |
| **Result** | : | Linear Model Prediction: biodegrades fast (probability of 0.5694)<br>Non-linear Model Prediction: does not biodegrade fast (probability of 0.1513)<br>Ultimate Biodegradation Timeframe: months (value = 2.2195)<br>Primary Biodegradation Timeframe: weeks (value = 3.1692)<br>MITI Linear Model Prediction: does not biodegrade fast (value = 0.272)<br>MITI Non-Linear Model Prediction: does not biodegrade fast (value = 0.0430) |
| **Reliability** | : | (2) valid with restrictions<br>Data were obtained by modeling. |

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### 3.6 BOD5, COD OR BOD5/COD RATIO

### 3.7 BIOACCUMULATION

| | | |
|---|---|---|
| **Elimination** | : | |
| **Method** | : | other |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

| | | |
|---|---|---|
| **Remark** | : | Inputs into the EPIWIN Program were a measured melting point of 45 degrees C, a CAS No. of 23500-79-0, and an emission rate to air of 0 kg/hr. |
| **Result** | : | The log bioconcentration factor (log BCF) is calculated [EPIWIN BCF Program (v2.14)] to be 2.945. |
| **Reliability** | : | (2) valid with restrictions<br>Data were obtained by modeling. |

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### 3.8 ADDITIONAL REMARKS

## 4.1 ACUTE/PROLONGED TOXICITY TO FISH

| | | |
|---|---|---|
| **Type** | : | other |
| **Species** | : | |
| **Exposure period** | : | 96 hour(s) |
| **Unit** | : | mg/l |
| **Limit test** | : | |
| **Analytical monitoring** | : | no |
| **Method** | : | other |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | EPIWIN ECOSAR (v0.99) was used to obtain the calculated LC50 value. Inputs to the model are CAS Number 23500-79-0 and the measured melting point (45 degrees C). |
| **Result** | : | The LC50 values were 0.3 or 0.118 mg/l, depending on whether the molecule was classified as a phenol or benzyl halide (respectively). |
| **Reliability** | : | (2) valid with restrictions<br>Data were obtained by modeling. |

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## 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

| | | |
|---|---|---|
| **Type** | : | other |
| **Species** | : | Daphnia sp. (Crustacea) |
| **Exposure period** | : | 48 hour(s) |
| **Unit** | : | mg/l |
| **Analytical monitoring** | : | no |
| **Method** | : | other |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | EPIWIN ECOSAR (v0.99) was used to obtain the calculated LC50 value. Inputs to the model are CAS Number 23500-79-0 and the measured melting point (45 degrees C). |
| **Result** | : | The LC50 values were 0.535 or 0.118 mg/l, depending on whether the molecule was classified as a phenol or benzyl halide (respectively). |
| **Reliability** | : | (2) valid with restrictions<br>Data were obtained by modeling. |

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## 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

| | | |
|---|---|---|
| **Species** | : | other algae: green |
| **Endpoint** | : | |
| **Exposure period** | : | 96 hour(s) |
| **Unit** | : | mg/l |
| **Limit test** | : | |
| **Analytical monitoring** | : | no |
| **Method** | : | other |
| **Year** | : | 2003 |
| **GLP** | : | no |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

| | | |
|---|---|---|
| **Remark** | : | EPIWIN ECOSAR (v0.99) was used to obtain the calculated LC50 value. Inputs to the model are CAS No. 23500-79-0 and the measured melting point (45 degrees C). |
| **Result** | : | The LC50 values were 0.13 or 0.118 mg/l, depending on whether the molecule was classified as a phenol or benzyl halide (respectively). |
| **Reliability** | : | (2) valid with restrictions<br>Data were obtained by modeling. |

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### 4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

### 4.5.1 CHRONIC TOXICITY TO FISH

### 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

### 4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

### 4.6.2 TOXICITY TO TERRESTRIAL PLANTS

### 4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

### 4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

### 4.7 BIOLOGICAL EFFECTS MONITORING

### 4.8 BIOTRANSFORMATION AND KINETICS

### 4.9 ADDITIONAL REMARKS

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

### 5.1.1 ACUTE ORAL TOXICITY

| | | |
|---|---|---|
| **Type** | : | LD50 |
| **Value** | : | = 7.71 ml/kg bw |
| **Species** | : | rat |
| **Strain** | : | Wistar |
| **Sex** | : | male |
| **Number of animals** | : | 10 |
| **Vehicle** | : | |
| **Doses** | : | 5 and 10 ml/kg |
| **Method** | : | other |
| **Year** | : | 1979 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Based on a specific gravity of 1.044 at 20 degrees C, the LD50 dose in g/kg is 8.04. |
| **Result** | : | Four animals treated with 10 ml/kg died; 2 between 6-24 hours of dosing and the others on days 2 or 3 after dosing. None of the animals exposed to 5 ml/kg died. The LD50 value calculated was 7.71 (5.71 to 10.4) ml/kg.<br><br>All animals had a sluggish, unsteady gait after 1 hour of treatment. All animals treated with 5.0 ml/kg recovered within 2 days. Two animals treated with 10 ml/kg were prostate 1 day after treatment. One of these animals recovered on day 2 (the other died on either day 2 or 3; see above). Survivors gained an average of 75 g over the course of the study.<br><br>Animals that died exhibited distended, gas-filled and injected stomachs, with glandular portions mottled pink and yellow; red kidney medullae; distended, liquid, blood-filled and injected intestines that were yellow and red in areas; and red adrenals. Survivors exhibited stomachs adhered to abdominal walls and livers at necropsy. |
| **Test condition** | : | Two groups of 5 nonfasted, male Hilltop-Wistar rats (90-120 g) were given 5.0 or 10.0 ml/kg test material by the oral route (presumably by gavage) as received. The length of the observation period after dosing is not clear (from 3-14 days); however, it probably was the standard 14 days since animals almost doubled their weight over the course of the experiment. All animals that died were subjected to gross necropsy. It is not clear when animals were terminated (from 3-14 days); however, they were necropsied at that time. The method of calculating the LD50 value was not listed. |
| **Test substance** | : | The test material was 80.5% pure. It is assumed that the material was the commercially isolated material that contains 11-13% methyl isobutyl ketone. It also contained 5.5% 6-t-butyl-2,4-dimethyl phenol. Other impurities were not identified. |
| **Reliability** | : | (2) valid with restrictions<br>The purity of the test material was not high. It is not known if doses were corrected for purity. The method of calculating the LD50 value was not listed. Only one sex was tested. |
| **Flag** | : | Critical study for SIDS endpoint |

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| | | |
|---|---|---|
| **Type** | : | LD50 |
| **Value** | : | > 2000 mg/kg bw |
| **Species** | : | rat |
| **Strain** | : | Sprague-Dawley |

| | | |
|---|---|---|
| **Sex** | : | male/female |
| **Number of animals** | : | 6 |
| **Vehicle** | : | other: dried arachis oil BP |
| **Doses** | : | 2000 mg/kg |
| **Method** | : | OECD Guide-line 423 |
| **Year** | : | 2000 |
| **GLP** | : | yes |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Result** : None of the animals died. Hunched posture and diarrhea were noted after treatment in all animals and lethargy and pilo-erection were found in males. Animals recovered 2-4 days after dosing. All animals gained a normal amount of weight over the observation period. No abnormalities were found at necropsy.

**Test condition** : The test material was freshly prepared as a suspension at 200 mg/ml in dried arachis oil BP. Homogeneity was assured by used of a Silverson homogenizer and vortex mixer. Animals [Sprague-Dawley Crl: CD(SD)IGSBR] were acclimated for at least 5 days before treatment. At the start of the study the males and females weighed 202 to 226 g and 216 to 230 g, respectively, and were approximately 8 weeks of age.

Animals were allowed free access to food and water with the exception of an overnight fast immediately before dosing and for approximately 3-4 hours after dosing. The diet, drinking water and bedding were routinely analyzed for contaminants that could affect the outcome.

Animals were housed in groups of 3/sex in rooms maintained at 19-25 degrees C, 30-70% relative humidity, and under a 12-hr light/dark cycle.

All animals (3 per sex) were dosed with 2000 mg/kg at a volume of 10 ml/kg by gavage. The volume administered was calculated according to the fasted body weight at the time of dosing (females 216 - 230 g and males 202 - 226 g). Females were dosed prior to males. Sufficient time was allowed between dosing to confirm the survival of previously dosed animals.

The animals were observed for death or overt signs of toxicity 0.5, 1, 2, and 4 hours after dosing and then daily for 14 days. Animals were weighed 7 and 14 days after treatment. Animals were killed by cervical dislocation 14 days after treatment. All animals were subjected to gross necropsies. External and internal (major organs) examinations were conducted. The appearance of any macroscopic abnormalities was recorded. No tissues were retained.

**Test substance** : The material was described as "purified A-1846". However, the exact purity of the material was not listed. The material was a white solid. According to a MSDS supplied by the manufacturer, unpurified material can contain 11-13% methyl isobutyl ketone. It is assumed that this material was removed during purification, since it is a liquid.

**Reliability** : (2) valid with restrictions
Only one dose was tested. The purity of the material is unknown.

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### 5.1.2 ACUTE INHALATION TOXICITY

| | | |
|---|---|---|
| **Type** | : | LC50 |
| **Value** | : | > 2000 ppm |
| **Species** | : | rat |
| **Strain** | : | |
| **Sex** | : | |
| **Number of animals** | : | 6 |

| | | |
|---|---|---|
| **Vehicle** | : | |
| **Doses** | : | |
| **Exposure time** | : | 4 hour(s) |
| **Method** | : | other |
| **Year** | : | |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | All 6 rats survived a 4-hour exposure to 2000 ppm (8.36 mg/l). |
| **Reliability** | : | (4) not assignable<br>There are not enough details to assign a reliability rating. |

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### 5.1.3 ACUTE DERMAL TOXICITY

| | | |
|---|---|---|
| **Type** | : | LD50 |
| **Value** | : | = 9.98 ml/kg bw |
| **Species** | : | rabbit |
| **Strain** | : | New Zealand white |
| **Sex** | : | male |
| **Number of animals** | : | 14 |
| **Vehicle** | : | |
| **Doses** | : | 0.8, 3.2, 6.4, 10.0 ml/kg |
| **Method** | : | other |
| **Year** | : | 1979 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Remark** | : | Based on a specific gravity of 1.044 at 20 degrees C, the LD50 dose in g/kg is 10.4. |
| **Result** | : | One animal treated with 3.2 ml/kg died on day 3. Two animals treated with 10.0 ml/kg died (one on day 3 and another on day 5). The LD50 value was 9.98 (4.41 to 22.6) ml/kg.<br><br>No clinical signs of systemic toxicity were noted. Surviving animals in all groups treated with 3.2 to 10 ml/kg lost weight over the course of the study. Erythema, edema and ecchymosis and areas of necrosis were noted at the test site in several animals over the course of the study (times at which these observations were recorded were not noted). Scabs were noted in an undetermined number of animals at 14 days. Gross necropsies of survivors were normal. The animals that died exhibited red kidneys. |
| **Test condition** | : | Skin of the 14 animals (avg wt. 2246 - 2543 mg/kg) was clipped prior to treatment. Undiluted test material was applied at 0.8 ml/kg to two rabbits and at 3.2, 6.4 and 10.0 ml/kg to 3 groups of 4 animals each. The application site was then covered for 24 hours. Animals were observed for 14 days and weighed prior to euthanization and necropsy. Animals that died also were subjected to necropsy. |
| **Test substance** | : | The test material was 80.5% pure. It is assumed that the material was the commercially isolated material that contains 11-13% methyl isobutyl ketone. It also contained 5.5% 6-t-butyl-2,4-dimethyl phenol. Other impurities were not identified. |
| **Reliability** | : | (2) valid with restrictions<br>The purity of the test material was not high. It is not known if doses were corrected for purity. The method of calculating the LD50 value was not listed. Only one sex was tested. |

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### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

### 5.2.1 SKIN IRRITATION

| | | |
|---|---|---|
| **Species** | : | rabbit |
| **Concentration** | : | undiluted |
| **Exposure** | : | Semiocclusive |
| **Exposure time** | : | |
| **Number of animals** | : | 6 |
| **Vehicle** | : | |
| **PDII** | : | 7 |
| **Result** | : | highly irritating |
| **Classification** | : | |
| **Method** | : | Draize Test |
| **Year** | : | 1979 |
| **GLP** | : | no data |
| **Test substance** | : | other TS |
| **Result** | : | The mean values for erythema at intact sites were 2.17 and 4.00 after 24 or 72 hours, respectively. For abraded sites, these scores were 2.50 and 4.00, respectively. The mean values for edema at intact sites were 3.50 and 4.00 after 24 or 72 hours, respectively. At abraded sites, these scores were 3.83 and 4.00, respectively. The primary irritation score was 7.00. The structure of the tissue at the site of contact was destroyed or changed irreversibly in 24 hours or less. |
| **Test condition** | : | Test material (0.5 ml) was applied under a covered patch to both intact and abraded sites (the number of sites was not stated). The contact time was not stated. Skin was evaluated 24, and 72 hours after application for erythema and edema. The study was conducted according to an "FHSA procedure" and reactions were scored according to the method of Draize et al., J Pharmacol Exper Ther 82:377, 1944. The maximum possible value for a skin reaction (excluding necrosis) was 4. The primary irritation score was the sum of the mean values divided by 4. |
| **Test substance** | : | The test material was 80.5% pure. It is assumed that the material was the commercially isolated material that contains 11-13% methyl isobutyl ketone. It also contained 5.5% 6-t-butyl-2,4-dimethyl phenol. Other impurities were not identified. |
| **Reliability** | : | (1) valid without restriction<br>The study was conducted according to an established method. |

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| | | |
|---|---|---|
| **Species** | : | rabbit |
| **Concentration** | : | undiluted |
| **Exposure** | : | no data |
| **Exposure time** | : | 4 hour(s) |
| **Number of animals** | : | 6 |
| **Vehicle** | : | |
| **PDII** | : | |
| **Result** | : | |
| **Classification** | : | |
| **Method** | : | other: DOT test |
| **Year** | : | 1980 |
| **GLP** | : | no data |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |
| **Result** | : | None of the 6 animals had necrosis. Therefore, the test material was not corrosive. No irritation scores were given. |
| **Test substance** | : | The test material was 80.5% pure. It also contained 5.5% 6-t-butyl-2,4-dimethyl phenol. Other impurities were not identified. |

| | | |
|---|---|---|
| **Reliability** | : | (4) not assignable<br>There are not enough details to assign a reliability rating. |

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### 5.2.2 EYE IRRITATION

| | | |
|---|---|---|
| **Species** | : | rabbit |
| **Concentration** | : | undiluted |
| **Dose** | : | .1 ml |
| **Exposure time** | : | |
| **Comment** | : | |
| **Number of animals** | : | 6 |
| **Vehicle** | : | |
| **Result** | : | highly irritating |
| **Classification** | : | irritating |
| **Method** | : | Draize Test |
| **Year** | : | 1979 |
| **GLP** | : | no data |
| **Test substance** | : | other TS |

| | | |
|---|---|---|
| **Result** | : | The average corneal, iridial and conjunctival scores at 24 hours were 28.3, 4.2 and 13.7, respectively. At 48 hours, these values were 21.7, 4.2 and 13.3, respectively. At 72 hours, they were 18.3, 0.8 and 11.7, respectively. At any of the readings made at 24, 48 and 72 hours there was: 1) discernable opacity or ulceration of the cornea other than a slight dulling of the normal luster, 2) inflammation of the iris other than slight deepening of the folds, or slight circumcorneal injection, 3) a diffuse, deep-crimson red appearance of the conjunctivae, with individual vessels not easily discernable, and 4) an obvious swelling of the conjunctivae excluding cornea and iris, with partial eversion of the lids. There also was tissue destruction or irreversible change of tissue in 24 hours or less. |
| **Test condition** | : | Test material (0.1 ml) was applied to eyes of 6 rabbits. Eyes were evaluated 24, 48 and 72 hours later. They do not appear to have been washed. The test was conducted according to an "FHSA procedure" and eyes were scored according to the method of Draize et al. (J Pharmacol Exper Ther 82:377, 1944). The maximum possible scores for eye irritation reactions (excluding necrosis) are cornea: 80; iris: 10; and conjunctivae:20. |
| **Test substance** | : | It is assumed that the material was the commercially isolated material that contains 11-13% methyl isobutyl ketone. |
| **Reliability** | : | (1) valid without restriction<br>The study was conducted according to an established method. |

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### 5.3 SENSITIZATION

### 5.4 REPEATED DOSE TOXICITY

### 5.5 GENETIC TOXICITY 'IN VITRO'

| | | |
|---|---|---|
| **Type** | : | Ames test |
| **System of testing** | : | S. typhimurium strains TA98, TA100, TA1535 and TA1537 and E. Coli WP2uvrA- |
| **Test concentration** | : | 5 to 1500 micrograms/plate for Salmonella strains; 50 to 5000 micrograms/plate for E. coli |

| | | |
|---|---|---|
| **Cytotoxic concentr.** | : | 500 micrograms/plate (without S-9) and 1500 micrograms/plate (with S-9) for Salmonella strains; 5000 micrograms/plate for E. coli |
| **Metabolic activation** | : | with and without |
| **Result** | : | negative |
| **Method** | : | OECD Guide-line 471 |
| **Year** | : | 2000 |
| **GLP** | : | yes |
| **Test substance** | : | as prescribed by 1.1 - 1.4 |

**Result** : The preliminary experiment revealed that the test material was toxic at concentrations > = 500 and 1500 micrograms/plate in strain TA100 without and with S-9, respectively. Although the background lawn was reduced somewhat in WP2uvrA- exposed to 5000 micrograms/plate (without S-9), toxicity was not considered to be excessive. Therefore, 1500 and 5000 micrograms/plate were the upper limits of concentrations in the mutation study with Salmonella and E. coli, respectively.

In both experiments, there was no significant increase in the number of mutants in any strains incubated with any concentration of test material (with or without S-9). All of the positive controls induced at least a 3-fold increase in the number of revertants. No precipitate was observed on the plates in the presence or absence of S-9. Spontaneous mutation rates in negative controls were acceptable.

**Test condition** : The Salmonella strains were obtained from the University of California at Berkeley, and E coli strain WP2uvrA- was obtained from the British Biological Research Association. Bacteria were stored frozen until used. Prior to use, characterization checks were carried out to confirm the amino-acid requirement, presence of rfa, R factors, uvrA or uvrB mutation and the spontaneous reversion rate. Overnight sub-cultures were prepared in nutrient broth and incubated at 37 degrees C for approximately 10 hours. Each culture was monitored spectrophotometrically for turbidity with titres determined by viable count analysis on nutrient agar plates.

The test material was weighed and approximate half-log dilutions prepared in dried dimethyl sulfoxide. A preliminary study using 0.15 to 5000 micrograms/plate was used to determine the toxicity of the material. Based on the results, the mutation study with the 4 Salmonella strains was conducted with 5, 15, 50, 150, 500, and 1500 micrograms/plate, and the study with E. coli was performed with 50, 150, 500, 1500 and 5000 micrograms/plate.

Measured aliquots (0.1 ml) of each of the bacterial cultures were dispensed into sets of test tubes followed by 2.0 ml of molten, trace histidine supplemented top agar, 0.1 ml of the test material formulation, vehicle or positive control [2, 3 or 5 micrograms/plate N-ethyl-N'-nitro-N-nitirosoguanidine (ENNG) for E. coli WP2uvrA- and Salmonella strains TA100 and TA1535 without S-9, respectively; 80 micrograms/plate 9-aminoacridine (AA) for strain TA1537 without S-9; 0.2 micrograms/plate 4-nitroquinoline-1-oxide (4NQO) for strain TA98 without S-9; 1 or 10 micrograms/plate 2-aminoanthracene (2AA) for Salmonella strain TA100 and E. coli WP2uvrA- with S-9, respectively; 2 micrograms/plate 2AA for strains TA1535 and TA1537 with S-9; and 5 micrograms/plate benzo(a)pyrene (BP) for strain TA98 with S9], and either 0.5 ml S9-mix or phosphate buffer. S-9 was prepared in-house from the livers of male Sprague-Dawley rats that had been orally induced with phenobarbitone/ beta-naphthoflavone. The contents of each test tube were mixed and equally distributed onto the surface of Vogel-Bonner Minimal agar plates (one tube per plate). The procedure was repeated in triplicate, for each bacterial strain and for each concentration of test material (with and without S-9 mix).

All plates were incubated at 37 degrees for approximately 48 hours and the

frequency of revertant colonies assessed using a Domino colony counter.

A second experiment was performed using the same test conditions as in the first.

An experiment was considered valid if all vehicle and untreated controls had numbers of spontaneous revertants within historical ranges, the appropriate characteristics of each tester strain were confirmed, all tester strain cultures had approximately 1 to 9.9 x 10E9 bacteria/ml before treatment, positive controls induced at least a 2-fold increase in revertants, there was a minimum of 4 non-toxic test material doses, and there was no evidence of excessive contamination.

A test material was considered positive in the assay if the material induced a reproducible, dose-related and statistically (Dunnett's method of linear regression) significant increase in revertants in at least one strain.

**Test substance** : The material was described as "purified A-1846". However, the exact purity of the material was not listed. The material was a white solid. According to a MSDS supplied by the manufacturer, unpurified material can contain 11-13% methyl isobutyl ketone. It is assumed that most of this material was removed during purification.

**Reliability** : (2) valid with restrictions
Purity of the test material was not listed.

**Flag** : Critical study for SIDS endpoint

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**Type** : Ames test
**System of testing** : S. typhimurium strains TA-98, TA-100, TA-1535, and TA-1537 and E. coli strain WP2uvrA-
**Test concentration** : 1000 micrograms/plate
**Cytotoxic concentr.** : 1000 micrograms/plate
**Metabolic activation** : with and without
**Result** : negative
**Method** : other
**Year** : 1978
**GLP** : no data
**Test substance** : as prescribed by 1.1 - 1.4

**Result** : The results of the tests were negative. Large zones of inhibition were present on all plates in the disc test.

**Test condition** : Test material was dissolved in ethanol. A disc test was performed on all strains and a plate test was performed on strains TA-1535 and TA-1537. The material was tested with and without metabolic activation. Only one dose was tested (1000 mg/plate or disc). No other study details were given.

**Test substance** : Purity of the test material was 90.1%. Impurities were not listed. The concentration tested was based on 100% active material.

**Reliability** : (4) not assignable
There are not enough details to assign a reliability rating.

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## 5.6 GENETIC TOXICITY 'IN VIVO'

## 5.7 CARCINOGENICITY

## 5.8.1 TOXICITY TO FERTILITY

### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

### 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

### 5.9 SPECIFIC INVESTIGATIONS

### 5.10 EXPOSURE EXPERIENCE

### 5.11 ADDITIONAL REMARKS

## 6.1 ANALYTICAL METHODS

## 6.2 DETECTION AND IDENTIFICATION

## 7.1 FUNCTION

## 7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

## 7.3 ORGANISMS TO BE PROTECTED

## 7.4 USER

## 7.5 RESISTANCE

## 8.1 METHODS HANDLING AND STORING

## 8.2 FIRE GUIDANCE

## 8.3 EMERGENCY MEASURES

## 8.4 POSSIB. OF RENDERING SUBST. HARMLESS

## 8.5 WASTE MANAGEMENT

## 8.6 SIDE-EFFECTS DETECTION

## 8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

## 8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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(2) Caterson C. 1978. Mutagenicity test report (Ames Salmonella test) for A-1846. Report Number M78-170 from CRD Division, Plastics Additives Department (Company ????)

(3) Cytec Industries, Inc. 2000. Material safety data sheet for A-1846, dated 10/30/2000. .

(4) Cytec Industries, Inc. 2003. Communication.

(5) Driscoll R. 2000. Purified A-1846 (CT-684-00). Acute oral toxicity in the rat - acute toxic class method. SafePharm Laboratories Limited Project Number 971/115 for Cytec Industries Inc., dated October 3.

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(13) Shaffer CB. 1980. Antioxidant A-1846 skin irritation test (D.O.T.). Carnegie-Mellon University Institute of Research Report No. 43-502 to American Cyanamid Company, dated January 31.

(14) Thompson PW. 2000. Purified A-1846 (CT-684-00). Reverse mutation assay "Ames Test" using Salmonella Typhimurium and Escherichia Coli. SafePharm Laboratories Limited Project Number 971/116 for Cytec Industries Inc., dated October 30.

## 10.1 END POINT SUMMARY

## 10.2 HAZARD SUMMARY

## 10.3 RISK ASSESSMENT